

## **SAS4A/SASSYS-1 Code Improvements for FY2016**

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**Nuclear Engineering Division**

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## ABSTRACT

SAS4A/SASSYS-1 is a simulation tool used to perform deterministic analysis of anticipated events as well as design basis and beyond design basis accidents for advanced reactors. This report summarizes ongoing tasks to modernize the SAS4A/SASSYS-1 code system to improve internal data management, update several other code modules, and add new features.

Code modernization activities focused on eliminating legacy data management in the balance-of-plant module, which was the only module that still used non-portable data allocation. Code extensions include the development of a new axial expansion model that can accurately account for non-uniform or heterogeneous fuel compositions. The most significant accomplishment is the addition of uncertainty quantification capabilities for transient simulations using the Dakota toolkit from Sandia National Laboratory.

The motivation for performing these updates stems from the relevance of SAS4A/SASSYS-1 to a number of U.S. Department of Energy programs as well as domestic and international collaborations. External collaborations have also produced improvements in the SAS4A/SASSYS-1 code, and these are summarized in this report. SAS4A/SASSYS-1 has a growing user base that continues to strengthen the promotion of advanced reactor concepts such as sodium cooled fast reactors. Additional users will help solidify DOE's leadership role in fast reactor safety both domestically and in international collaborations.



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## 1 Introduction

SAS4A/SASSYS-1 is a simulation tool used to perform deterministic analysis of anticipated events as well as design basis and beyond design basis accidents for advanced liquid-metal-cooled nuclear reactors.[1] With its origin as SAS1A in the late 1960s, the SAS series of codes has been under continuous use and development for over forty-five years and represents a critical investment in safety analysis capabilities for the U.S. Department of Energy. This report documents fiscal year 2016 activities that were carried out to modernize and to improve the modeling capabilities in SAS4A/SASSYS-1. Improvements include updating the data management for the balance of plant (BOP) steam system models, extending the axial thermal expansion models to account for non-uniform or heterogeneous fuel compositions, and coupling SAS4A/SASSYS-1 with Dakota[2] to provide extensive transient uncertainty quantification and optimization capabilities. This report satisfies the deliverable for the Level 3 milestone M3AT-16AN1702034, "SAS4A/SASSYS-1 Improvements." A separate report, ANL-ART-74, addresses the Level 2 milestone M2AT-16AN1702032, "Coupling the System Analysis Module with SAS4A/SASSYS-1." [3]

Continued modernization and improvement of the SAS4A/SASSYS-1 code system are motivated by the relevance of its simulation capability to a number of U.S. Department of Energy programs as well as domestic and international collaborations. In FY16 version 5.1 was released. In addition, a limited version, referred to as "Mini SAS," was made available at no cost for non-commercial use. Mini SAS is compiled from the same source used to compile SAS4A/SASSYS-1, but the sodium boiling and severe accident modeling capabilities are excluded and the code is limited to modeling only five core channels. Active programs and collaborations that currently use SAS4A/SASSYS-1 include the following:

- EBR-II IAEA Benchmark: The DOE-NE Advanced Reactor Concepts program is supporting a high-profile Coordinated Research Project with the International Atomic Energy Agency based on the Shutdown Heat Removal Tests conducted at EBR-II. Both protected (SHRT-17) and unprotected (SHRT-45R) loss-of-flow tests are part of the benchmark activity. SAS4A/SASSYS-1 models of both tests have been developed to provide results under the CRP.
- FFTF Benchmark: Pacific Northwest National Laboratory is preparing benchmark specifications for the Passive Safety Tests (PST) carried out at the Fast Flux Test Facility between 1984 and 1986. The most prominent tests were the loss of flow without scram (LOFWOS). In collaboration with PNNL, Argonne National Laboratory is assessing the benchmark specifications and preparing SAS4A/SASSYS-1 models for verification and validation purposes.
- GAIN Voucher Program: Oklo, Inc. is one of the recipients of a Gateway for Accelerated Innovation in Nuclear award. Under the award, Oklo is gaining access to knowledge of metallic alloy fuel. They are also investigating the available tools for fast reactor analysis and have acquired a license for Mini SAS version 5.1.
- NEUP Projects: Several Nuclear Energy University Program awards are utilizing SAS4A/SASSYS-1 or Mini SAS as part of their scope of work. The University of California at Berkeley is using Mini SAS to evaluate safety benefits that might be achieved with autonomous reactivity control devices. Other universities are

preparing experiments that can improve the modeling of thermal stratification in sodium-cooled fast reactors, with the goal that the improved models would be incorporated into SAS4A/SASSYS-1.

- RTDP: Under the Regulatory Technology Development Plan, the U.S. DOE is identifying and addressing gaps for the licensing of SFRs. One such gap is the regulatory acceptability of SFR analysis tools. Initial efforts are underway to establish more rigorous software quality assurance practices for SAS4A/SASSYS-1.
- GE-Hitachi Nuclear Energy Americas, LLC has a government-use license for SAS4A/SASSYS-1 to carry out development of modern probabilistic risk assessment evaluations of the PRISM reactor concept. GEH and Argonne National Laboratory are collaborating on this work under the 2014 Advanced Reactor Research and Development funding opportunity (DE-FOA-0001163).
- ASTRID Collaboration with CEA: An implementation agreement has been established between the U.S. DOE and the Commissariat à l'énergie atomique et aux énergies alternatives of France for cooperation in low carbon energy technologies. One purpose of the agreement is to evaluate the safety performance of the ASTRID reactor design. DOE will accomplish this using the SAS4A/SASSYS-1 safety analysis code.
- CIAE Bilateral Collaboration: The DOE-NE Office of International Nuclear Energy Policy and Cooperation has established the U.S.–China Bilateral Civil Nuclear Energy Cooperative Action Plan (BCNECAP) with the China Institute of Atomic Energy. Joint activities under the action plan include model development and safety analyses of the China Experimental Fast Reactor using SAS4A/SASSYS-1.
- TerraPower TWR Reactor Concept: TerraPower, LLC has licensed the SAS4A/SASSYS-1 source code to perform safety analysis studies for their “Traveling Wave Reactor” concept. TerraPower also funds code development activities that improve the modeling capabilities of SAS4A/SASSYS-1.
- KAERI PG-SFR: The Korean Atomic Energy Research Institute acquired a license for SAS4A/SASSYS-1 to perform safety analysis and model development for the “Prototype Generation-IV Sodium Fast Reactor”. KAERI is supporting metallic fuel severe accident model developments that will be incorporated into a future version of SAS4A/SASSYS-1.
- KINS: The Korea Institute of Nuclear Safety is an independent regulatory expert organization that supports the Nuclear Safety and Security Commission (NSSC) in Korea. KINS recently acquired a license for SAS4A/SASSYS-1 to support the regulatory obligations over the PG-SFR project.
- KTH ELECTRA LFR Concept: The Royal Institute of Technology (Kungliga Tekniska Högskolan) in Stockholm Sweden has a license for SAS4A/SASSYS-1 to perform natural circulation design performance studies of their ELECTRA lead-cooled fast reactor concept.
- JAEA Bilateral Collaboration: The Civil Nuclear Energy Research and Development Working Group (CNWG) was established by the U.S.-Japan Bilateral Commission on Civil Nuclear Cooperation in 2012 to enhance coordination of joint civil nuclear research and development efforts. The Japan Atomic Energy Agency and Argonne

National Laboratory plan to collaborate under the CNWG to improve the oxide fuel severe accident modeling capabilities in SAS4A/SASSYS-1.

- NRA: The Nuclear Regulation Authority of Japan has acquired a license for SAS4A/SASSYS-1. The NRA plans to use SAS4A/SASSYS-1 to support the relicensing evaluation of Monju.

During FY16, fourteen new license agreements were established for Mini SAS and SAS4A/SASSYS-1 (see Table 1).

Improvements to the SAS4A/SASSYS-1 code that were completed in FY2016 are summarized in the next section. Then, a brief summary of related work supported by third-party users is provided to give a broader perspective on overall SAS4A/SASSYS-1 developments. The current distributed version of SAS4A/SASSYS-1 is 5.1. Many of the recent updates, supported by both DOE and third-party users, will be included in the upcoming release of version 5.2.

Table 1: SAS License Agreements Established during FY2016.

Organization	Version	Purpose
Massachusetts Institute of Technology	Mini SAS 5.1	NEUP Project
Purdue University	Mini SAS 5.1	Academic Use
University of California, Berkeley	Mini SAS 5.1	NEUP Project
Qvist Atomenergi AB	Mini SAS 5.1	NEUP Project
China Institute of Atomic Energy	SAS4A/SASSYS-1 5.1	BCNECAP/CEFR
Ulsan National Institute of Science and Technology (UNIST)	Mini SAS 5.1	Academic Use/ PG-SFR
University of Illinois	Mini SAS 5.1	NEUP Project
Texas A&M University	Mini SAS 5.1	Academic Use/ NEUP Proposal
Virginia Commonwealth University	Mini SAS 5.1	NEUP Project
Pacific Northwest National Laboratory	SAS4A/SASSYS-1 5.1	FFTF Benchmark
University of Michigan	Mini SAS 5.1	Academic Use
Oklo, Inc.	Mini SAS 5.1	GAIN Voucher
Kansas State University	Mini SAS 5.1	NEUP Project
Japan Nuclear Regulation Authority	SAS4A/SASSYS-1 5.1	Monju Licensing

## 2 Code Improvements

### 2.1 Balance of Plant Data Management

SAS4A/SASSYS-1 was originally developed for computing architectures with extremely limited memory capacities compared to current hardware. Early code development practices revolved around minimizing memory usage. A fundamental strategy was to overlay, or reuse, the same memory locations for multiple models. The strategy for modernizing data management in SAS4A/SASSYS-1 was developed in FY2013 [4] and has been implemented over time.

The balance of plant (BOP) model, which was one of the last remaining modules utilizing outdated data management techniques, has been updated to adopt the modern strategy. One of the key goals was to remove references to steam generator and super-heater allocated memory that incurred array bound violations. In doing this, advanced compiler options for identifying array bounds violations or uninitialized variables can now be utilized throughout the code.

A new BOP data module has been created which contains new data types and various subroutines for reading, writing, and moving BOP data. Models and functionality of the BOP remains unchanged. The new data structure, which represents all steam generator, super-heater, and associated conservation equation matrix variables, replaces the allocated BOP container that formerly required array bound violations for access. As such, the subroutine *POINST* has been updated to remove the dynamically allocated BOP pointers and the subroutine *POINS2*. Additionally *DYNALL*, which had been reduced by previous updates to handle only BOP data, has been eliminated as BOP memory container allocation is no longer necessary. In addition to creation of the new BOP data structure, steam generator and super-heater named common block definitions (e.g. SGEN1, SGENS1, PRM4CM, etc.) have been migrated to new data modules.

Several subroutines have been created (e.g. *LoadSG*, *StoreSG*, *UpdateSG*, etc.) for transferring steam generator and super-heater data between the respective named common blocks (e.g. SGEN1, SGENS1, etc.) and the new data structure. These subroutines replace older data swapping methods and are intended to be more transparent and encapsulated relative to the previous subroutines. Rather than utilizing array aliasing and bounds violations, the new data structure is copied directly in the modernized subroutines. Table 2 provides a listing of the superseded subroutines.

It should be noted that during testing and debugging of the BOP revisions, it was necessary to modify the BOP scratch file designation for the file fort.8. Rather than automatically deleting the scratch file at the end of a simulation, it is retained. This is needed to support a restart simulation that uses the BOP models.

Table 2: BOP Subroutine Updates

Original	Updated	Comments
MVPPSG	LoadSG StoreSG	Unique load and store subroutines created to increase code readability and error checking.
MVPPSH	LoadSH StoreSH	Unique load and store subroutines created to increase code readability and error checking.
SHIFT0	UpdateSG	Rewritten to remove equivalence use and improve clarity.
SHIFTS	UpdateSH	Rewritten to remove equivalence use and improve clarity.

In modernizing the BOP data management framework, an issue with the maximum number of BOP steam generators was identified that could lead to errantly overwriting input data in PMR4IN. Specifically, the LoadSG and StoreSG subroutines (and the legacy MVPPSG and MVPPSH subroutines) handle BOP steam generator data in the common blocks (SGEN1, SGEN2, SGEN3,) and data derived from PMR4IN input (locs 3934-4173). While the BOP allows for a maximum of eight steam generators, PMR4IN input space is allotted for only four steam generators. If more than four steam generators are invoked in a BOP model, PMR4IN input beyond location 4173 will be overwritten during the data swap. In order to address this issue, a check on the number of steam generators has been added to SSPRM4 which will trigger the graceful termination of the code if the steam generator limit is violated.

## 2.2 Heterogeneous Axial Expansion

The basic axial expansion model in SAS4A/SASSYS-1 implicitly assumes a uniform axial fuel composition within a channel. This is not the case for novel core concepts that include explicit heterogeneities, such as the ASTRID low-void worth core with an internal blanket. Nor is it the case with a long-lived core that develops implicit heterogeneities due to breeding in the upper and lower portions of the fuel and considerable depletion near the mid plane.

In the traditional axial expansion model, a single vector, FUELRA, represents the fuel worth in each channel as a function of axial position. FUELRA is defined on the initial, steady-state fuel mesh. As fuel expands, fuel material can leave one mesh location and enter an adjacent location with a different worth (see Figure 1). The difference in worth by location provides the reactivity feedback contribution due to axial expansion of the fuel. Algebraically, this can be written as

$$\begin{aligned}\Delta\rho_{\text{fuel}} &= \rho'_{\text{fuel}} - \rho_{\text{fuel}} = \int \mu'(z)R(z)dz - \int \mu(z)R(z)dz \\ &= \int [\mu'(z) - \mu(z)]R(z)dz\end{aligned}$$

where  $\rho$  is the fuel reactivity,  $\mu(z)$  is the original linear fuel density (kg/m) and  $\mu'(z)$  is the expanded (or contracted) linear fuel density.  $R(z)$  is the piecewise flat fuel worth defined by FUELRA.

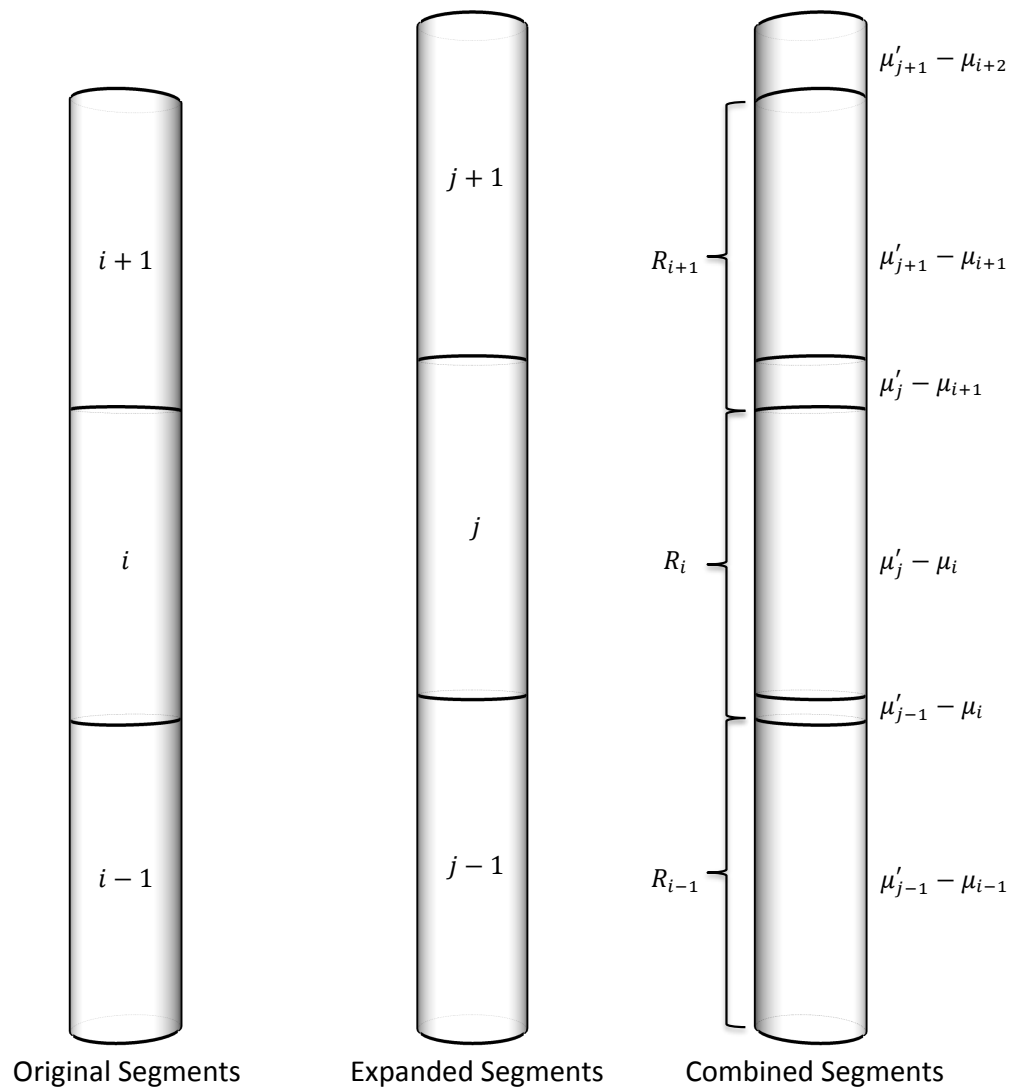


Figure 1: Comparison of original and perturbed segments as a result of thermal expansion.

Movement of fuel mass leads to reactivity changes because the fuel worth,  $R_i$ , is on a fixed mesh but the linear fuel density,  $\mu$ , is changing.

Depending on the nature of the fuel expansion or contraction, the combination of overlapping segments from the original and perturbed geometries could be fairly complex. One way to view the overlap is to define the matrix  $\Delta\mathbf{Z}$ , where element  $i, j$  corresponds to the length of the overlap between the axial segments:

$$\Delta\mathbf{Z} = \begin{bmatrix} \Delta z_{1,1} & \Delta z_{1,2} & \cdots & \Delta z_{1,n} \\ \Delta z_{2,1} & \Delta z_{2,2} & & \vdots \\ \vdots & & \ddots & \vdots \\ \Delta z_{n,1} & \cdots & \cdots & \Delta z_{n,n} \end{bmatrix}$$

$\Delta z_{i,j}$  corresponds to the extent that axial segment  $j$  in the perturbed geometry occupies axial segment  $i$  in the original geometry. With no expansion, the matrix is diagonal where the diagonal elements correspond to the original axial segment heights. For small expansions or contractions, the matrix will be tri-diagonal. Assuming the reactivity worth distribution is piecewise flat on the original geometry, the above integrals can be rewritten in matrix form:

$$\begin{aligned} \rho'_{\text{fuel}} &= \int R(z)\mu'(z)dz \\ &= \mathbf{R}^T \Delta\mathbf{Z} \boldsymbol{\mu}' \end{aligned}$$

and

$$\begin{aligned} \rho_{\text{fuel}} &= \int R(z)\mu(z)dz \\ &= \mathbf{R}^T \Delta\mathbf{Z}_0 \boldsymbol{\mu} \end{aligned}$$

where  $\Delta\mathbf{Z}_0$  is the unperturbed diagonal matrix.

Since most of the terms in the  $\Delta\mathbf{Z}$  matrix are likely to be zero, it would be inefficient to calculate them all. Fortunately it is not necessary. Given two vectors for the original and perturbed segment boundaries,  $\mathbf{z}$  and  $\mathbf{z}'$  respectively, the following algorithm will suffice:

```

ρ' = 0
i = 1
do: j = 1 ... J
  ρj = 0
  while: i ≤ I
    Δz = min(zi+1, z'j+1) - max(zi, z'j)
    if (Δz > 0): ρj = ρj + RiμjΔz
    if (zi+1 ≥ z'j+1): exit-while
    i = i + 1
  end-while
  ρ' = ρ' + ρj
end-do

```

In the above algorithm,  $J$  is the total number of fuel segments, and  $I$  is the number of entries in the reactivity feedback table. This corresponds to a  $\Delta\mathbf{Z}$  matrix with dimensions

( $I, J$ ). In the traditional implementation,  $I = J = MZ$  and the fixed point of fuel expansion is at the bottom of the pin, so the original and perturbed geometries always align at that point. In the new model, the clause “if ( $\Delta z > 0$ )” allows for arbitrary alignment. The  $i$  or  $j$  indices will advance until an overlapping region is found, if one exists.

If a fuel pin has an axially heterogeneous composition, then the single vector RAFUEL is insufficient. In the new model, two matrices are defined: 1) *mfFuel* defines the mass fraction of each fuel component as a function of axial position, and 2) *raData* defines the reactivity worth for each fuel component as a function of axial position. To extend the model further, the assumption that the reactivity worth table falls on the same mesh as the fuel is dropped and an *raMesh* vector is added to the input. This allows tremendous flexibility for reactor physics analyses because perturbation theory calculations no longer have to be adapted to the same mesh used by SAS4A/SASSYS-1.

With some modifications, the above algorithm can be updated to handle multiple fuel components within a single pin, each with its own reactivity feedback distribution.

```

 $\rho' = 0$ 
do:  $k = 1 \dots N$ 
   $i = 1$ 
  do:  $j = 1 \dots J$ 
     $\rho_j = 0$ 
    while:  $i \leq I$ 
       $\Delta z = \min(z_{i+1}, z'_{j+1}) - \max(z_i, z'_j)$ 
      if ( $\Delta z > 0$ ):  $\rho_j = \rho_j + R_i^k f_j^k \mu_j \Delta z$ 
      if ( $z_{i+1} \geq z'_{j+1}$ ): exit-while
       $i = i + 1$ 
    end-while
     $\rho' = \rho' + \rho_j$ 
  end-do
end-do

```

where  $N$  represents the number of fuel components in the pin,  $f_j^k$  is the mass fraction of component  $k$  in fuel segment  $j$ , and  $R_i^k$  is the worth of component  $k$  in the unperturbed segment  $i$ .

In the new model there is no limit to the number of fuel components that can be defined for each channel, and there is no limit to the level of detail that can be defined for the reactivity feedback distribution. In terms of input, the new model requires the following:

TABLE FUELRA

Height	Comp_A	Comp_B	Comp_C	(etc.)
$\Delta z_1$	$R_1^A$	$R_1^B$	$R_1^C$	
$\Delta z_2$	$R_2^A$	$R_2^B$	$R_2^C$	
...				
$\Delta z_I$	$R_I^A$	$R_I^B$	$R_I^C$	
END				

```

TABLE FUELMF
      Comp_A      Comp_B      Comp_C      (etc.)
       $f_1^A$        $f_1^B$        $f_1^C$ 
       $f_2^A$        $f_2^B$        $f_2^C$ 
      ...
       $f_J^A$        $f_J^B$        $f_J^C$ 
END

```

where  $\Delta z_i$  defines the reactivity feedback mesh (raMesh),  $R_i^k$  defines the reactivity worth per kilogram for component  $k$  of fuel (raFuel), and  $f_j^k$  defines the mass fraction of component  $k$  in the fuel (mfFuel) at each axial position.

Extensive input validation is performed. For example, every fuel mass fraction vector must have a corresponding reactivity worth vector. The number of axial entries for the fuel mass fraction table must match the number of fuel segments in the channel. Finally, the new model does allow the “Height” column to be omitted. In this case, the code assumes the mesh for the reactivity worth is the same as for the fuel.

## 2.3 Transient Uncertainty Quantification

### 2.3.1 Overview

Advancements in the knowledge of nuclear reactor performance have led to an increased need to perform Sensitivity Analyses (SA) and Uncertainty Quantification (UQ) in the advanced reactor domain. The role of uncertainty quantification spans many facets in the nuclear industry, including system design and optimization, licensing, and probabilistic risk assessment.[5] In FY15, the capability to perform uncertainty quantification of a system-level safety analysis for Sodium-cooled Fast Reactors (SFR) was established by coupling SAS4A/SASSYS-1 with RAVEN and preliminary work began to couple SAS4A/SASSYS-1 with Dakota.[6] In FY16 the coupling with Dakota was completed and evaluated.

The Design Analysis Kit for Optimization and Terascale Applications (Dakota) software is an uncertainty quantification and optimization toolkit developed and supported by Sandia National Laboratories (SNL) [2]. Development of Dakota began in 1994, and was primarily focused on optimization applications. The software is written largely in C++ and Perl, and utilizes several SNL-developed and noncommercial libraries and packages, which are distributed with Dakota as necessary.

In FY16, a Python interface was developed to couple Dakota with SAS4A/SASSYS-1. The Dakota executable is available pre-compiled via the SNL Dakota website and was coupled with SAS4A/SASSYS-1 through a black-box interface. Dakota invokes a simulation code by either direct linkage or a system call. During the system call, the external code is initialized and data communication between Dakota and the external code occurs through parameter and response files. Because the system call is more straightforward, it was applied to invoke SAS4A/SASSYS-1 simulations in this study.

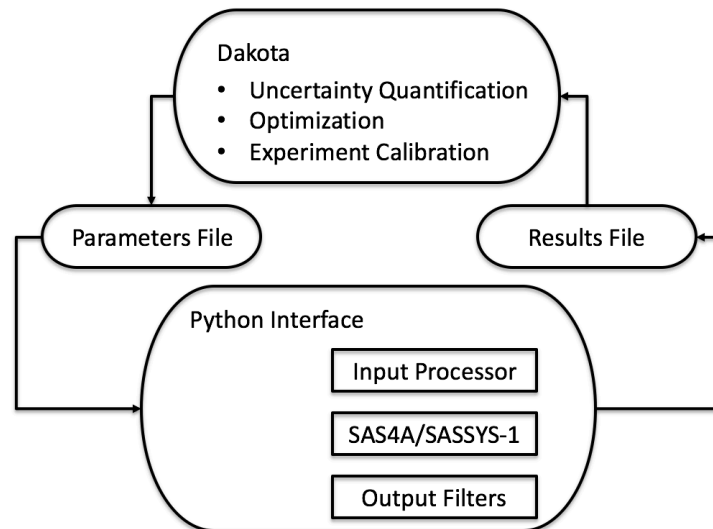


Figure 2: Dakota-SAS4A/SASSYS-1 Coupling Scheme

A coupled simulation proceeds as follows: uncertain parameters in a template SAS4A/SASSYS-1 input file are replaced with values generated by Dakota, this unique input file is used to run a SAS4A/SASSYS-1 simulation, and the response values of interest from the SAS4A/SASSYS-1 simulation are saved for post-processing by Dakota. Figure 2 illustrates this coupling scheme.

A Dakota input file defines the sampling/optimization methods (including bounds and distribution type for all variables), uncertain parameters, interface strategy, and system code responses, or key output variables, for the coupled simulation being performed. The sampling method or optimization functions are identified in the method section. Uncertain variables, probability distributions, and upper and lower bounds are specified in the variable section. The interface section defines the driver file name, the parameter file for the parameters randomly generated by Dakota, the SAS4A/SASSYS-1 template input file, and the response file saving the SAS4A/SASSYS-1 simulation results. The interface searches for the uncertain variables in the input template file and replaces them with the values generated by Dakota to create a new SAS4A/SASSYS-1 input. The total number of responses is specified as Dakota input, and the target responses along with the selection criteria are specified in the Python interface.

After the SAS4A/SASSYS-1 simulation concludes, the Python interface converts the binary output files (PRIMAR4.dat and CHANNEL.dat) into CSV files and searches for the target responses. The present interface has four output filters for the simulation results from SAS4A/SASSYS-1: 'max' for the maximum value, 'min' for the minimum value, 'begin' for the beginning value of the simulation, and 'end' for the ending value of the simulation. Users choose the channels on which the filters are applied. If the channels are not specified, the interface will search for the target through all channels in the system.

The responses of interest are written in a result file and returned to Dakota for quantification of the statistical metrics. Means, standard deviations, and 95% confidence intervals are computed for each of the responses. In addition, Dakota calculates the most

common statistics between uncertainties and responses of interest, such as the covariance, Pearson coefficient, simple, partial, and rank correlations. The Pearson coefficient is a measure of the linear correlation between two variables and its value is in a range between +1 to -1, inclusive. A Pearson coefficient with a large absolute value means that two variables are strongly correlated. A positive Pearson coefficient means positive correlation while a negative value indicates that the two variables are inversely proportional.

In cases where the uncertain parameters are correlated, a correlation matrix is implemented in the Dakota-SAS4A/SASSYS-1 interface such that the uncertainties will be perturbed together according to the matrix. An N-dimensional vector  $\vec{i}$  is generated by Dakota, where each of the elements in vector  $\vec{i}$  is a Dakota-generated value based on the user-specified distribution. Then, vector  $\vec{i}$  is mapped to an M-dimensional vector  $\vec{j}$  via the  $M \times N$  correlation matrix  $A$ . The vector  $\vec{j}$  contains the elements that will be used as SAS4A/SASSYS-1 inputs. For example, reactivity feedback coefficients are correlated by nuclear data uncertainties. The method developed for the correlated uncertainties was applied to propagate the nuclear data uncertainty on ASTRID safety performance.[7] The correlation matrix  $A$  represents the covariance of the reactivity coefficients and the vector  $\vec{j}$  includes the spatially-dependent reactivity coefficients that will be used in transient simulation.[8] In addition to the correlation matrix, the uncertain variables can also be characterized by complicated algebraic expressions (e.g. power, logarithmic, trigonometric functions).

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} i_1 \\ \vdots \\ i_n \end{bmatrix} = \begin{bmatrix} j_1 \\ \vdots \\ j_m \end{bmatrix}$$

Dakota is capable of performing parallel simulations by launching multiple SAS4A/SASSYS-1 jobs concurrently. Two options are supported by Dakota for parallelism. Dakota execution is launched on a single processor with multiple cores and control does not return until all the simulations are completed and the response files have been written. This is appropriate for PCs with a multi-core processor. In addition, a parallel launch utility is available for executing Dakota across multiple processors. Parallel configurations can be reallocated for each interface in a multi-model study. Each processor is usually assigned with one task and Dakota can use the message passing routines based on the MPI standard to communicate data between processors. In terms of multi-level parallelism on a massively parallel computing platform, Dakota seems more robust than RAVEN.

### 2.3.2 Uncertainty Quantification Capabilities

After coupling Dakota and SAS4A/SASSYS-1, the new capability to perform uncertainty quantification was demonstrated for an advanced reactor systems level safety analysis. The primary sampling techniques supported by Dakota are Monte Carlo sampling, Latin Hypercube Sampling (LHS), and Grid sampling. These basic sampling techniques are simple and straightforward approaches for uncertainty propagation. Since SAS4A/SASSYS-1 simulations are not computationally expensive, adequate sampling can be performed in a reasonable amount of time given moderate resources. Nevertheless, when a large number of uncertainties are investigated simultaneously or the understanding of complex reactor

system is incomplete, the number of evaluations required by these basic sampling techniques quickly becomes prohibitive and more advanced uncertainty quantification methods are required. In addition to these basic sampling techniques, Dakota supports more robust methods for uncertainty propagation, including the Reliability Method and the Importance Sampling method for failure analyses. In FY16, both the basic and advanced methods were tested using ABTR transients.

#### *2.3.2.1 Conventional Sampling-based Techniques*

In FY15, SAS4A/SASSYS-1 was coupled with RAVEN and a demonstration of the uncertainty quantification of advanced reactors was published in Reference [9]. In FY16, the Dakota-SAS4A/SASSYS-1 package was applied to repeat the previous uncertainty quantification analyses. Both RAVEN and Dakota support the following three sampling techniques: Grid sampling, Monte Carlo (MC) sampling, and Latin Hypercube Sampling (LHS). Figure 3 illustrates these sampling techniques.

- In the Grid sampling approach, an N-dimensional grid is discretized into segments and each dimension represents an uncertain variable. Sampling is performed at each node of the grid and therefore all possible combinations of the uncertain variables are evaluated. The number of sample points required by grid sampling depends exponentially on the input dimensions.
- The Monte Carlo method involves a random sampling based on a specific distribution between the lower and upper bounds on each of the input variables. This is the most straightforward approach for uncertainty propagation.
- Latin Hypercube Sampling (LHS), a specialized version of the Stratified approach in RAVEN, is a method that explores the input space where the uncertain domain is subdivided into N segments. The relative length of each segment is determined by the probability distribution of the corresponding uncertainty. Every subgroup of the uncertain variable is randomly assigned to a sample only one time. There is no restriction on the number of bins for each uncertainty, but LHS requires all uncertain variables to have the same number of bins. The total number of samples equals the number of bins for each variable. According to the Dakota manual, LHS technique requires fewer samples than the MC method for the same statistical accuracy.

The uncertainty quantification of the ABTR unprotected loss of heat sink (ULOHS) transient was performed with the coupled RAVEN-SAS4A/SASSYS-1 package in FY15. The same activity was repeated using the Dakota-SAS4A/SASSYS-1 package to benchmark the two coupled packages. The ULOHS transient is initiated when heat rejection through the power conversion system is lost and the reactor scram system fails to operate. In the SAS4A/SASSYS-1 model for the ULOHS transient, the intermediate pumps trip and heat rejection through the steam generator is reduced to zero simultaneously. The primary loop pumps do not trip and continue to operate at full speed throughout the simulation.

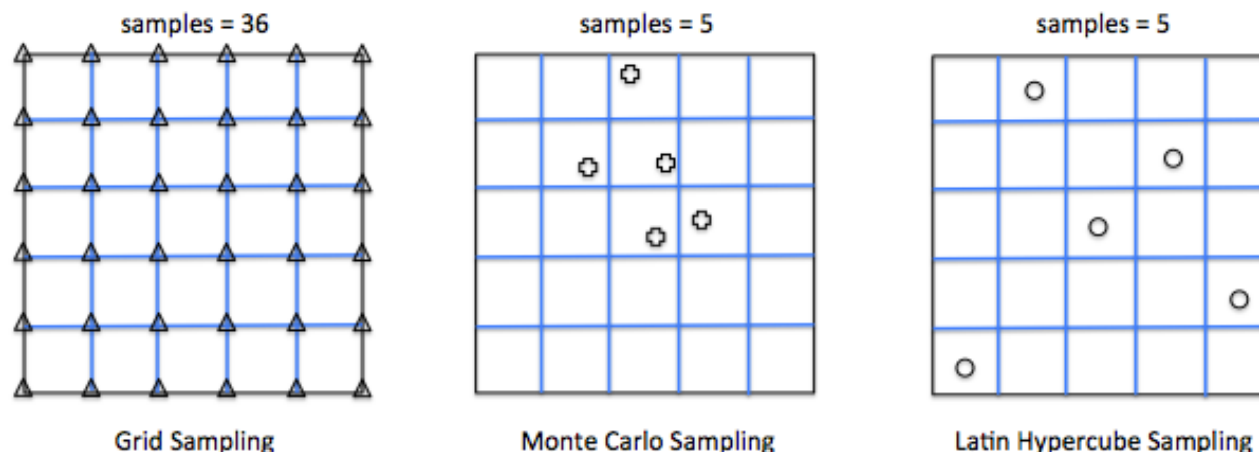


Figure 3: Sampling Techniques Implemented in RAVEN and Dakota

The uncertain variables considered in the benchmark include:

- Control rod drive thermal expansion coefficient
- Control rod expansion feedback coefficient
- Doppler feedback coefficient
- Radial expansion feedback coefficient
- Multiplication of reactor vessel length and expansion coefficient

The variables above are assumed to be uniformly distributed within 25% of their nominal values, which are shown in Table 3. MC sampling and LHS techniques were applied in Dakota with 250 samples. The peak fuel temperature during the ABTR ULOHS transient was selected as the response of interest.

The statistics generated from RAVEN and Dakota are compared in Table 4 and Table 5 lists the Pearson coefficients. The results for the two uncertainty quantification toolkits are in good agreement. As expected, the MC and LHS techniques can achieve the same accuracy as the grid sampling technique with a much smaller population. Because radial core expansion contributes a large negative feedback during the ULOHS transient, a small change of the radial expansion feedback coefficient will impose a large effect on the net reactivity feedback. Therefore, both RAVEN and Dakota show a large positive Pearson value for the radial expansion feedback coefficient. Figure 4 and Figure 5 show the impacts of the uncertainties on the peak fuel temperatures during the ABTR ULOHS transient.

Table 3: Nominal Values of Uncertain Parameters for ABTR ULOHS Transient

Uncertain Parameters	Nominal
Vessel Length and Expansion Coefficient	$1.46 \times 10^{-4}$ m/K
Control Rod Drive Thermal Expansion Coefficient	$2.0 \times 10^{-5}$ K <sup>-1</sup>
Control Rod Expansion Feedback Coefficient	-24.0 \$/m
Doppler Feedback Coefficient	$-1.37 \times 10^{-3}$ \$/m
Radial Expansion Feedback Coefficient	$-4.17 \times 10^{-3}$ \$/K

Table 4: Uncertainty Quantification of the Peak Fuel Temperature from RAVEN and Dakota

	RAVEN-SAS4A/SASSYS-1		Dakota-SAS4A/SASSYS-1	
	Grid	MC	MC	LHS
Samples	2000	250	250	250
Mean	822.8	823.0	822.7	822.8
Std. Dev.	1.27	1.19	1.18	1.19
Skewness	0.26	0.17	0.17	0.16
Kurtosis	2.23	-0.87	-1.09	-1.12
Cumulative Distribution Function for 5%	820.8	821.0	821.0	821.0
Cumulative Distribution Function for 95%	825.6	825.0	824.6	824.8

Table 5: Comparisons of the Pearson Coefficients for Peak Fuel Temperature in ABTR ULOHS

Uncertain Parameters	RAVEN-SAS4A/SASSYS-1		Dakota-SAS4A/SASSYS-1	
	Grid	MC	MC	LHS
Vessel Length and Exp. Coefficient	0.09	0.14	0.10	0.08
Control Rod Drive Thermal Exp. Coeff.	-0.22	-0.12	-0.19	-0.21
Control Rod Exp. Feedback Coefficient	0.12	0.14	0.12	0.15
Doppler Feedback Coefficient	0.05	0.12	0.03	0.02
Radial Exp. Feedback Coefficient	<b>0.96</b>	<b>0.96</b>	<b>0.97</b>	<b>0.97</b>

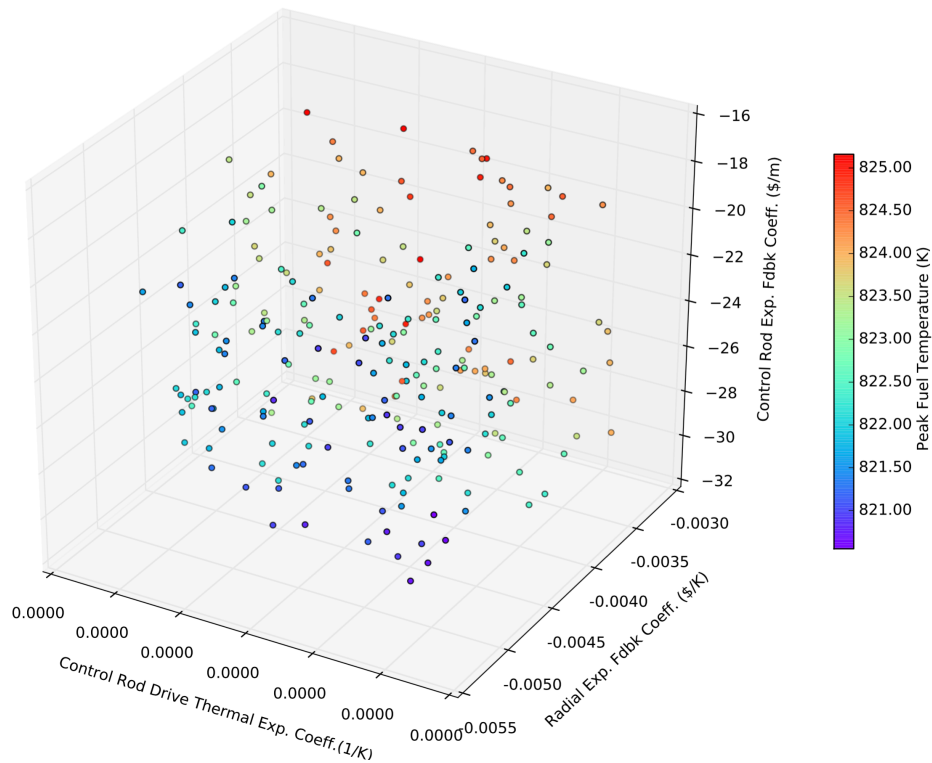


Figure 4: Effects of the Three Most Important Uncertainties in Reactivity Feedback on Peak Fuel Temperature during ABTR ULOHS Transient by MC Sampling

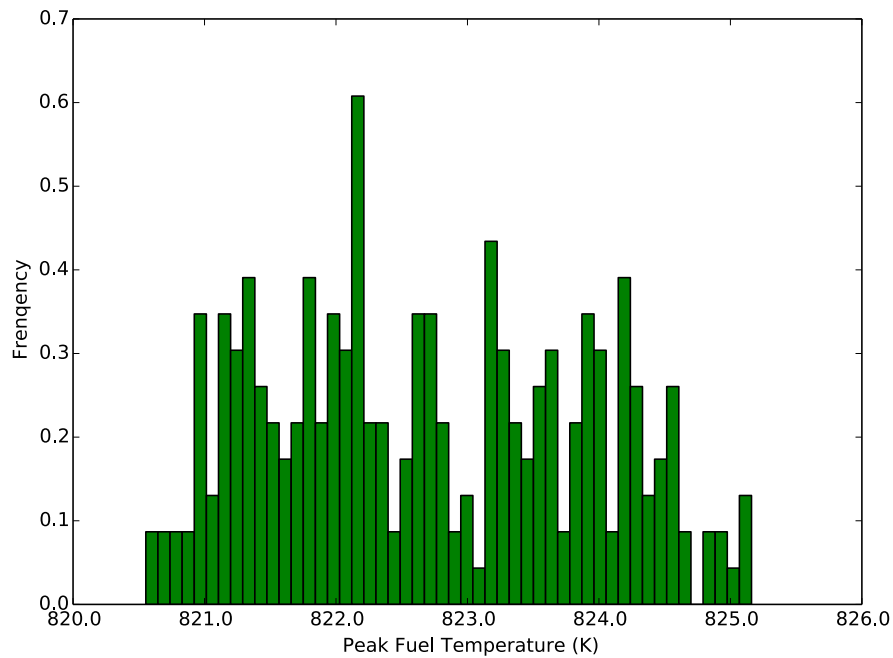


Figure 5: Distribution of Peak Fuel Temperature during ABTR ULOHS Transient by MC Sampling

### 2.3.2.2 Reliability Method

The Reliability Method provides an alternative approach to the conventional sampling-based techniques when uncertainty quantification analyses are computationally demanding. The algorithm of the Reliability Method was developed to compute the statistics in the tails of the response distribution in a more efficient way than sampling-based approaches. The Reliability Method addresses the problem to locate the most probable points and integrate the approximate probabilities. Given a set of uncertain variables and specified distributions, the probability that the response function is below or above a certain level is calculated. In advanced nuclear system safety analyses, the Reliability Method can be applied to identify the region of interest where the design constraints are satisfied. The cumulative distribution function (CDF) of the safety characteristics, such as boiling margin, can be calculated by the Reliability Method.

An ABTR unprotected transient overpower (UTOP) scenario was used to demonstrate the Reliability Method enabled by the Dakota-SAS4A/SASSYS-1 package. The UTOP transient occurs in ABTR if one or more inserted control rods are accidentally withdrawn and the reactor scram systems fails. In the demonstration case for the Reliability Method, it is assumed that external reactivity of between 0.1 and 0.7 \$ is added to the core over a period of between 5 and 100 seconds. Uniform distributions are applied for both uncertainties. The margins to coolant boiling are considered here as the response of interest. The Reliability Method in Dakota generates the approximate values of the cumulative distribution functions for prescribed response levels in a range from 420K to 485K, as shown in Figure 6. Based on the uncertainty distributions and their upper/lower bounds, the probability that the minimum coolant boiling margin is less than 420 K during the ABTR UTOP transient is expected to be 28.4%.

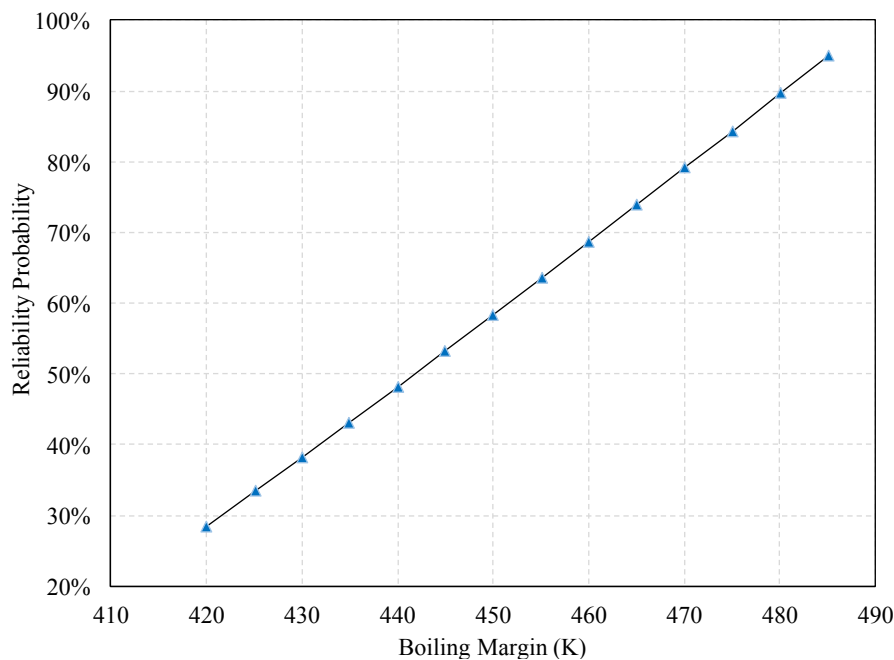


Figure 6: Reliability Probability of the Coolant Boiling Margin for ABTR UTOP Transient by the Reliability Method

### 2.3.2.3 Importance Sampling Method

The Importance Sampling provides another method to estimate the failure probabilities in a more efficient way than the traditional sampling-based techniques. This method preferentially samples important regions of the failure region of interest, and then appropriately weights the samples to obtain an unbiased estimate of the failure probability. The Importance Sampling method is expected to be applicable for advanced nuclear systems with limited safety margins, such as the ASTRID design concept during an Unprotected Loss of Supply Station Power (ULOSSP) transient.[10] Instead of a large number of response function evaluations, which would be required for conventional sampling-based methods, the Importance Sampling method reduces the computational cost by sampling near the failure region on the uncertain domain.

The ABTR UTOP transient described in Section 2.3.2.2 was used to demonstrate the Importance Sampling method supported by Dakota-SAS4A/SASSYS-1. As with the reliability analysis, it is assumed that an external reactivity of between 0.1 and 0.7\$ is added to the core and over a period of 5 to 100 seconds. Uniform distributions are applied for both uncertainties. A failure region where the boiling margin is less than 400 K was selected for demonstration purposes and problem simplification. The Importance Sampling method involves two steps: an initial Latin Hypercube sampling is performed to generate the importance density shown as the background, then successive samples are centered around the points near the failure region. As shown in Figure 7, the Importance Sampling preferentially focuses on the area where the boiling margin is below 400K. Given the specified uncertainty domain, a failure probability of 10.5% is computed.

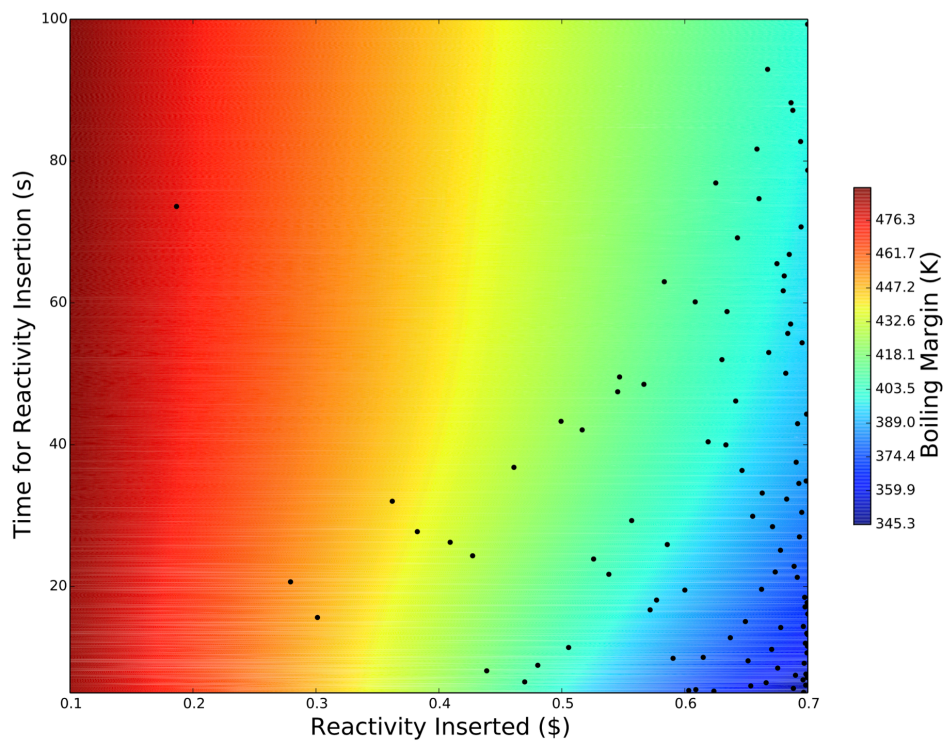


Figure 7: Importance Sampling Approach for Boiling Margin Below 400K

### 2.3.3 Other Capabilities

Dakota provides capabilities in two additional areas that are not reported here but that have been tested and demonstrated with SAS4A/SASSYS-1. The two areas are optimization and calibration.

Dakota utilizes a variety of optimizers to minimize (or maximize) objective functions while satisfying user-defined constraints. The coupled Dakota and SAS4A/SASSYS-1 capability was tested in FY16 for design optimization, which has the potential to improve the state of advanced reactor safety analyses. The primary approaches available in Dakota are gradient-based and derivative-free methods. Gradient-based optimizers are the most efficient way to navigate to a local optimum in situations where gradients can be computed analytically and efficiently. Since the derivatives of the simulation results from SAS4A/SASSYS-1 are not available, the gradient-based approach is not applicable for the design optimization by Dakota-SAS4A/SASSYS-1 package.

Derivative-free methods were tested to demonstrate the automated optimization capability. The Pattern Search (PS) and Evolutionary Algorithm (EA) methods were applied for the local and global optimum of SAS4A/SASSYS-1 results, respectively. In order to reduce the computational cost for a global optimum, a hybrid method combining the pattern search and evolutionary algorithm methods was tested as well.

Model calibration capabilities were also evaluated. Similar to optimization, Dakota can calibrate uncertain user-defined input to better match experimental results. For example, sensitivity studies show that uncertainty in radial expansion, control-rod driveline expansion, and cold pool mixing have large impacts on the simulation results for several EBR-II benchmark tests. Because there are large uncertainties in the parameters for these models, Dakota can adjust the parameters to produce simulations results that have better agreement with experimental observations.

The Dakota calibration feature is capable of evaluating the objective responses from multiple models simultaneously. This allows Dakota to determine a single set of input parameters that applies to several different transient conditions or experiments. Having this capability provides valuable insight that can be used to prioritize model developments.

### 2.4 Resolved Code Issues

Although the majority of code developments focused on improved data management and new capabilities, a small number of issues were identified and addressed in FY2016:

- Improved support for compiling on Linux (x86) systems by reducing the need for non-portable code to deal with legacy data management. SAS4A/SASSYS-1 is supported on all major x86 platforms: Mac OS, Windows, and Linux.
- Improved the handling of long lines in the extended input processor. This also provides additional verification of input while reading input TABLE blocks.
- Corrected an issue in the input processor and the Control System parser that would assume a decimal-point location for formatted floating point input that did not have an explicit decimal point.

- SAS4A/SASSYS-1 now offer users a warning about illegal tab-characters when reading fixed formatted input.
- Resolved an issue with cubic interpolation where some coefficients were not properly initialized depending on compiler options. The coefficients are now initialized with correct values regardless of compiler options.
- Resolved an issue where a divide-by-zero error could occur in the new Control System. The new input signal for channel flow rate is now properly initialized during steady state.

### 3 Related Work

#### 3.1 TerraPower – Control System Updates

Significant contributions to SAS4A/SASSYS-1 development are supported by TerraPower, LLC under a sponsored research agreement. The goal of the work was to devise, implement, and document changes to the Control System module to provide access to channel-dependent data such as coolant, cladding, and structure temperatures. Although the Control System had broad access to numerous plant state variables, it had limited access to core channel data other than inlet and outlet temperatures and flows.

Table 6: New Core Channel Sensors Available in SAS4A/SASSYS-1

- |                               |                                  |
|-------------------------------|----------------------------------|
| • Fuel Centerline Temperature | • Coolant Inlet Temperature      |
| • Fuel Average Temperature    | • Coolant Inlet Pressure         |
| • Fuel Surface Temperature    | • Coolant Inlet Flow Rate        |
| • Clad Inner Wall Temperature | • Coolant Outlet Temperature     |
| • Clad Midwall Temperature    | • Coolant Outlet Pressure        |
| • Clad Outer Wall Temperature | • Coolant Outlet Flow Rate       |
| • Coolant Temperature         | • Pin Bundle $\Delta T$          |
| • Coolant Pressure            | • Pin Bundle $\Delta P$          |
| • Coolant Saturation          | • Assembly $\Delta T$            |
| • Coolant Boiling Margin      | • Assembly $\Delta P$            |
| • Coolant Average Temperature | • Assembly Power                 |
| • Structure Inner Temperature | • Linear Power                   |
| • Structure Outer Temperature | • Peak Linear Power              |
| • Reflector Inner Temperature | • Fission Gas Plenum Temperature |
| • Reflector Outer Temperature | • Fission Gas Plenum Pressure    |
| • Peak Fuel Temperature       |                                  |
| • Peak Clad Temperature       |                                  |
| • Peak Coolant Temperature    |                                  |
| • Minimum Boiling Margin      |                                  |

The new Control System module is a nearly complete rewrite of the previous implementation. The module is built around object-oriented constructs such as class inheritance and polymorphism. These concepts allow the Control System to be written as a generic data acquisition system and extension to new signal inputs is very straightforward.

In addition to existing signals (plant state variables), a user now can utilize the numerous core channel *sensors* in their control system logic (see Table 6). These sensors can be queried by the Control System at any axial location for any channel. This capability provides tremendous flexibility in defining complex control system logic.

### **3.2 Regulatory Technology Development Plan**

A key component of reactor design commercialization in the U.S. is the completion of a license application approved by the Nuclear Regulatory Commission, where approval is contingent on, among other things, satisfactory demonstration of the design basis and response to transient and accident scenarios using accepted codes and methods. Following the recommendations of a licensing research plan by Sandia National Laboratory [12] and the Regulatory Technology Development Plan by Idaho National Laboratory,[13] a task has been launched to systematically develop SFR safety analysis codes and methods that will be used in a licensing framework. SAS4A/SASSYS-1 was identified as a key safety analysis code for SFRs as it is one of the only integrated systems level tools that treats the range of steady-state and transient phenomena that must be characterized in a license application.

Subsequent efforts in FY16 have been centered on development of a quality assurance (QA) framework for SAS4A/SASSYS-1 that can meet the appropriate regulatory guidance and other QA requirements (DOE, NQA-1, etc.). Much of this work is being executed in accordance with guidance from Oak Ridge National Laboratory provided in a related deliverable.[14] Efforts are underway to develop a Quality Assurance Plan, Configuration Management Plan, and associated procedures (Software Testing, Error Reporting and Corrective Actions, Feature Change, Version Release, and Coding Standards and Requirements) specific to SAS4A/SASSYS-1. It is expected that this provisional framework will be extended to other SFR codes in future efforts.

Work in this area will continue in FY17 for SAS4A/SASSYS-1, with finalization and implementation of the provisional QA framework, addition of unit tests, creation of additional V&V test problems, expansion of line coverage of the V&V test suite, and implementation of an automated regression test suite.

### **3.3 NEAMS System Analysis Module**

In contrast to the heritage of SAS4A/SASSYS-1, the SFR System Analysis Module, SAM, is a more recent development sponsored by the DOE-NE Office of Advanced Modeling and Simulation (NEAMS). Although a relatively new effort, significant accomplishments have been achieved through the use of modern software design and development practices.

SAS4A/SASSYS-1 contains a capable primary and intermediate system modeling component, PRIMAR-4. PRIMAR-4 can represent complex arrangements of coolant system components including pumps, piping, valves, intermediate heat exchangers, air dump heat exchangers, and steam generators. SAS4A/SASSYS-1 also contains a control system module

that can dynamically interact with PRIMAR-4 based on user-defined logic and controls. Control signals can affect certain plant state parameters such as scram reactivity, pump speed, and valve actuation.

In addition to its capabilities, PRIMAR-4 has some shortcomings. The most significant shortcomings are in the form of data management, code structure, and user input limitations. Outdated code structure makes extension of the PRIMAR-4 module more difficult, and the user input format for PRIMAR-4 limits the number of volumes and segments that can be used to describe a given system.

A separate effort is underway to couple SAM to SAS4A/SASSYS-1.[3] SAM will provide an alternative to PRIMAR-4 for primary, secondary, and decay heat coolant system modeling capabilities. Despite the advanced modeling capabilities in SAM, it will initially be somewhat limited in the system components and phenomena that can be represented. For example, component models for electromagnetic pumps and multi-layer stratified volumes have not yet been developed. Nor is there support for a balance of plant model.

Nevertheless, the modern software design of SAM should facilitate rapid development of models and continued investment by NEAMS would eliminate these gaps.

Until SAM matures to provide the same range of components and phenomena that PRIMAR-4 provides, PRIMAR-4 will be the preferred module for primary and intermediate coolant systems modeling. By completing the coupling, however, a path forward will be available to support enhanced modeling capabilities that are not currently possible.

## 4 Summary

Modernization of the data management in SAS4A/SASSYS-1 and extensions to include new capabilities will ensure that SAS4A/SASSYS-1 remains a viable simulation tool for the safety analysis of advanced, non-LWR reactor concepts, particularly sodium fast reactors. In FY16 the data management for the balance-of-plant (BOP) module was replaced with modern data structures, a new model for heterogeneous axial expansion was implemented to support a broader scope of designs, and the code was coupled to the powerful uncertainty quantification tool Dakota.

SAS4A/SASSYS-1 continues to have a growing user base with fourteen new licensees in FY16. It is also a critical component to a number of DOE programs as well as domestic and international collaborations. The continued use and expanding user base will strengthen the promotion of advanced reactor concepts such as sodium cooled fast reactors.

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